Contamination Free O Kα Spectrum Emitted from MgO

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INTRODUCTION

Pronounced chemical bonding effects of two types are observed in X-ray emission spectra when an electron fills an inner-shell vacancy localized on a valence band. One is fine structure originating from molecular orbital components on the valence band, and the other is a difference in X-ray satellite intensities caused by emission from multiply ionized states. However, these emission features have almost the same energies and they can not be observed separately without a tunable monochromator. The Advanced Light Source (ALS) is a powerfultool for separating these spectra - by employing excitation energies large enough for single ionization but too small for multiple ionization. X-ray emission spectra from light elements that are free from the satellites caused by multiple ionization are fascinating targets for study because they reflect the electronic structure of the valence band. In the present study, an observed O Kα spectrum emitted from MgO has been compared with a theoretical spectrum derived from the discrete variational (DV) Xα molecular orbital (MO) calculation.

EXPERIMENTAL RESULTS and MO CALCULATIONS

O Kα emission spectra of MgO shown in Fig.1 were measured using a grating spectrometer at B.L.8. Excitation energies are written in the figure (a-g). Spectra noted as a and d are magnified in the left-hand figure. The Raman scattered peaks shift to high energy sides if high excitation energies are employed, and then the Raman peaks are overlapped with MO peaks at ~522eV and ~525eV when photons with less energies than 533eV are used for excitation. On the other hand photons with higher energies than 555eV produce the satellite noted as K^1L^1 on the 580eV excitation spectrum. Here K^1L^1 denotes a satellite emitted from a state with one K- and one L-shell vacancies. This means that the spectrum excited with 539eV photons is free from the Raman and the satellite peaks, and then can simply be explained by a MO scheme. Both

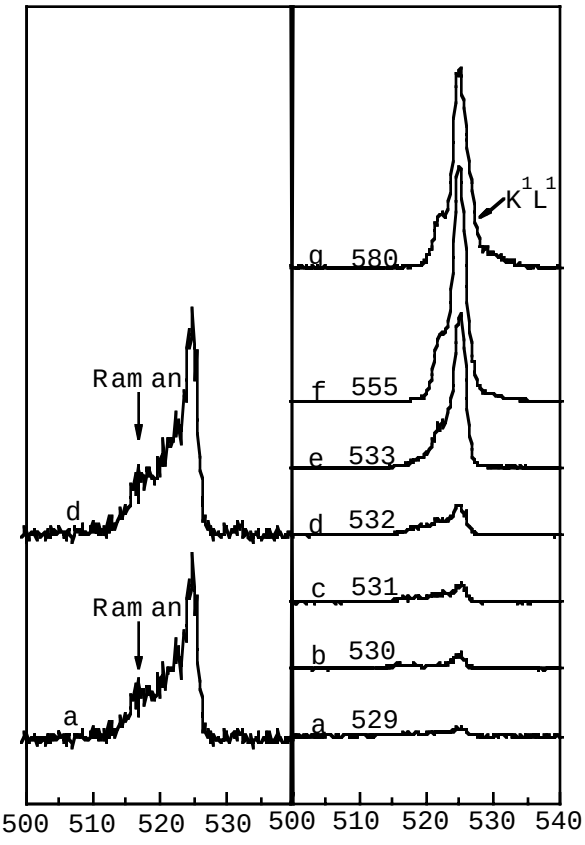

Fig. 1 O Kα emission spectra from MgO

experimental and theoretical spectra are compared with each other, as shown in Fig.2, and their conformity is satisfactory. Here the DV-Xα MO calculations[1),2)] were carried out under the conditions of 1) basis sets for O and Mg: 1s~3p, 2) a well potential: $0.7a_0$ in width and -3.0 Hartree in depth, 3) sample points: 2000. Now a_0 is an interatomic distance between Mg and O.

FURTHER APPLICATION

Similar spectra were taken from CaO and SrO, which were compared with theoretical ones as shown in Fig. 3. Agreement between them is unsatisfactory. On the low energy sides of the observed spectra a weak shoulder or a peak can clearly be seen. To confirm the validity of the theoretical spectra, O Kα emission spectra of CaO and SrO were reexamined by x-ray fluorescence (XRF) spectrometry. If CaO and SrO were exposed to air for a few hours, O Kα spectra with a weak peak at ~522 eV were recorded (unfortunately 7th reflection of Ca Kα is overlapped with the main peak of O Kα for CaO). This means that difference in the shape of O Kα spectra is expected to be seen among MgO, CaO and SrO, if surface of these chemical compounds are clean.

REFERENCES

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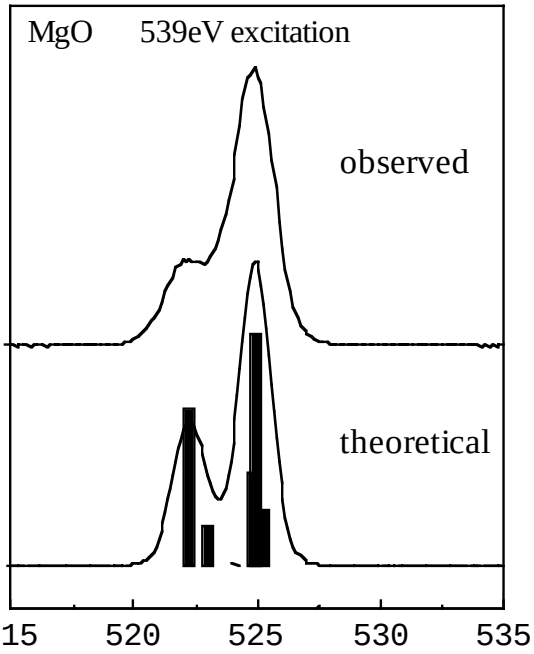

Fig. 2 Comparison between observed O Kα free from Raman and satellite spectra, and theoretical 2p density of states calculated by the DV-Xα method for MgO

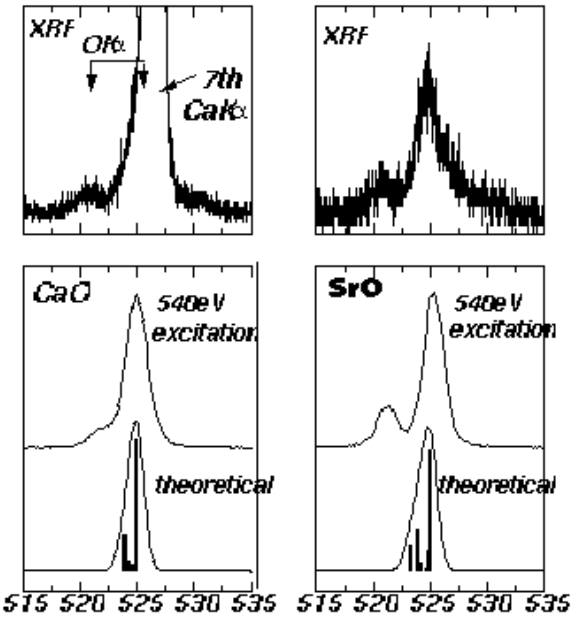

Fig. 3. O Kα XRF spectrum from CaO and SrO (top) which were exposed to air for a few hours. Observed Kα from CaO and SrO at ALS BL 8.0 and theoretical 2p density of states calculated with the DV-Xα method are shown in bottom figures.